2,2-Bis(bromomethyl)-1,3-propanediol 3296-90-0 | DTXSID9020164

Model Performance

N.A. I. I.	D .
Model	II)ata
IVIOGCI	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 288 °C

Global applicability domain: Inside

Local applicability domain index: 3.57e-01

Confidence level: 6.51e-01

Nearest Neighbors from the Training Set

Image not found

Tetraethylene glycol Measured: 328 Predicted: 318

Image not found

Sobrepin Measured: 271 Predicted: 260

Image not found

1,4-Cyclohexanedimethanol

Measured: 285 Predicted: 278

Image not found

Triethylene glycol Measured: 285 Predicted: 278